1-Nitrododecane

Other names:	Dodecane, 1-nitro-
Inchi:	InChI=1S/C12H25NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13(14)15/h2-12H2,1H3
InchiKey:	MQEMKUTWMALMCC-UHFFFAOYSA-N
Formula:	C12H25NO2
SMILES:	CCCCCCCCCCCC[N+](=O)[O-]
Mol. weight [g/mol]:	215.33
CAS:	16891-99-9

Physical Properties

Property code	Value	Unit	Source
gf	85.71	kJ/mol	Joback Method
hf	-301.77	kJ/mol	Joback Method
hfus	38.20	kJ/mol	Joback Method
hvap	58.90	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.184		Crippen Method
mcvol	197.360	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
tb	625.80	K	Joback Method
tc	812.93	K	Joback Method
tf	368.61	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.52	J/mol×K	625.80	Joback Method
cpg	551.82	J/mol×K	656.99	Joback Method
cpg	567.33	J/mol×K	688.18	Joback Method
cpg	582.06	J/mol×K	719.37	Joback Method
cpg	596.06	J/mol×K	750.56	Joback Method
cpg	609.34	J/mol×K	781.75	Joback Method
cpg	621.94	J/mol×K	812.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45334e+01
Coeff. B	-4.75054e+03
Coeff. C	-9.96520e+01
Temperature range (K), min.	433.12
Temperature range (K), max.	614.78

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16891999&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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